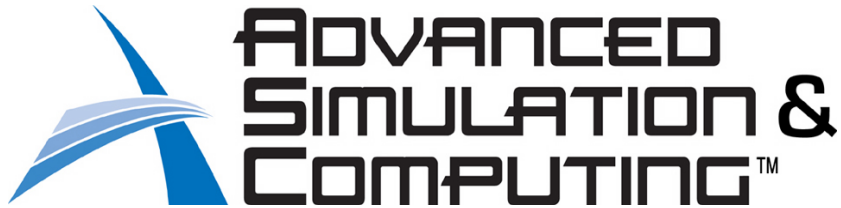
Predictive Science Academic Alliance Program (PSAAP)

The slides that follow were presented at the PSAAP Bidder's Meeting May 16-17, 2006 and represent the ASC Trilab authors and interests as presented in the associated White Paper for this subject area.



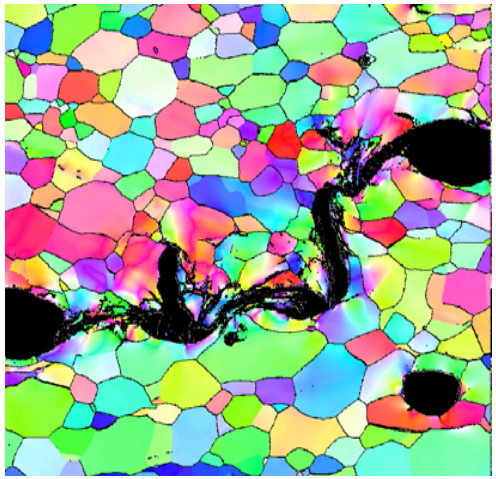
Material Damage and Failure

Er-Ping Chen (SNL)
Curt Bronkhorst (LANL)
Kimberly Budil (LLNL)

NNSA ASC Predictive Science Academic Alliance Program Bidders Meeting
16 May, 2006

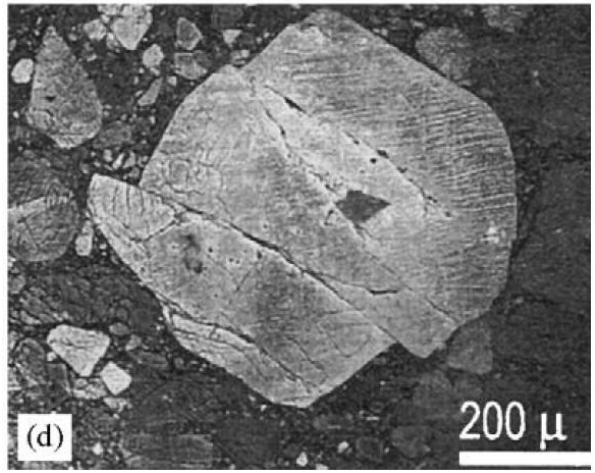
LA-UR-06-3418

Overview



Ductile Damage & Failure

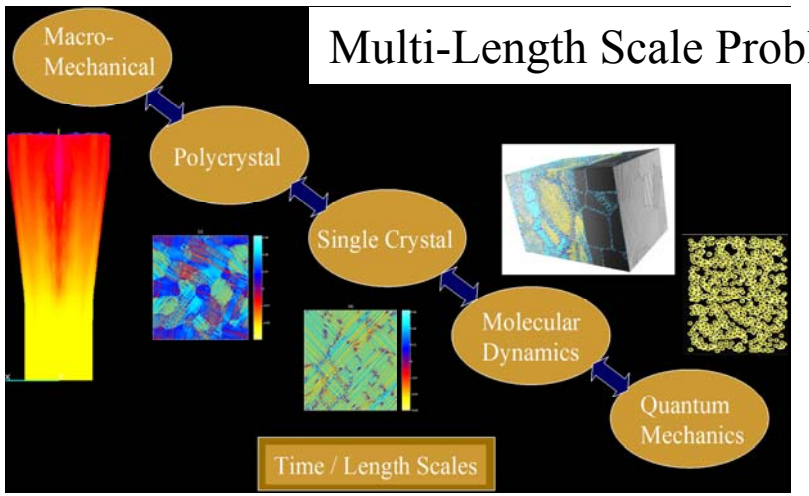
Brittle Damage & Failure



Tantalum, B. Henrie

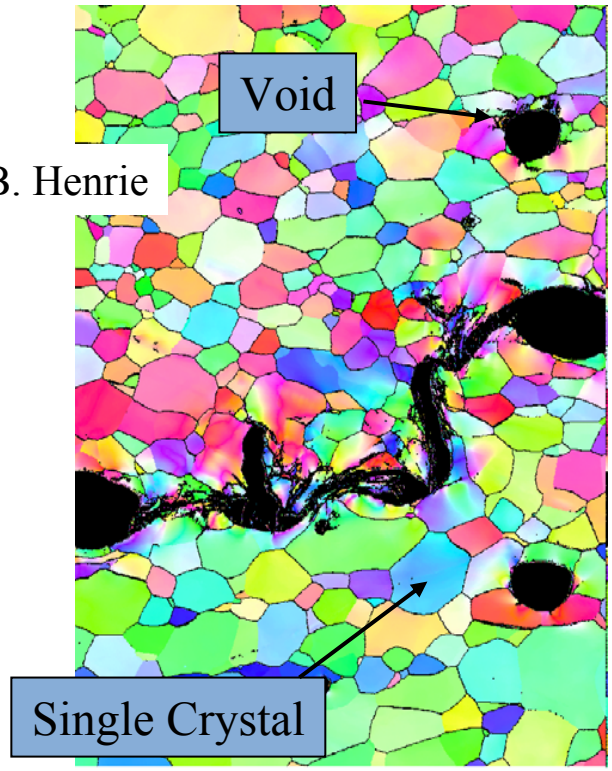
HMX, Dienes et al., 2006

Multi-Length Scale Problem



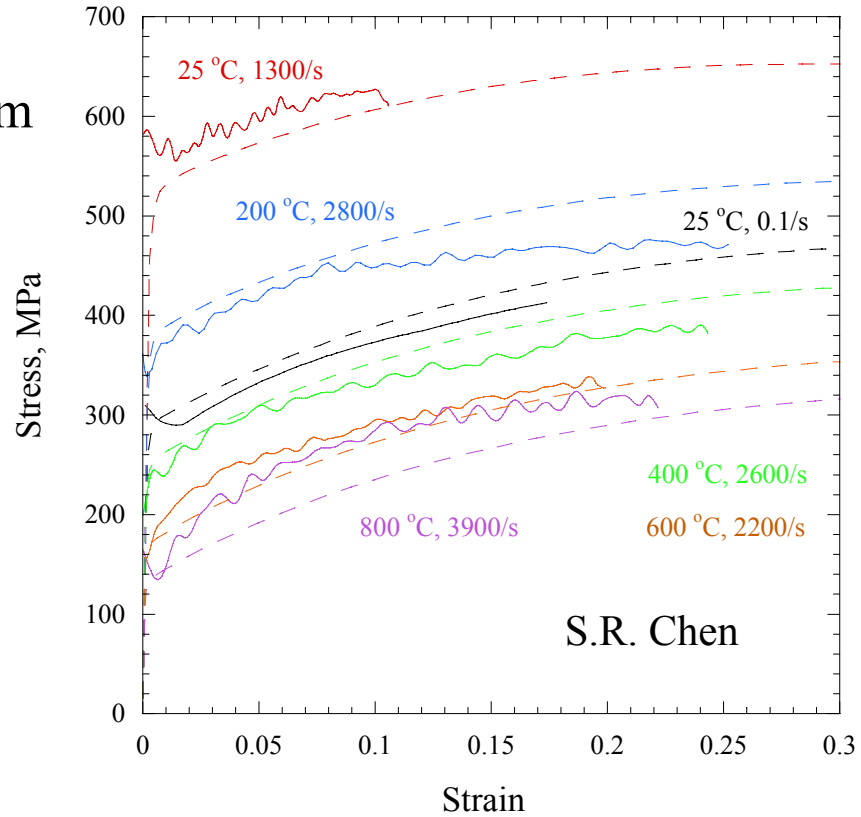
F. Addessio

Ductile Behavior



B. Henrie

Tantalum

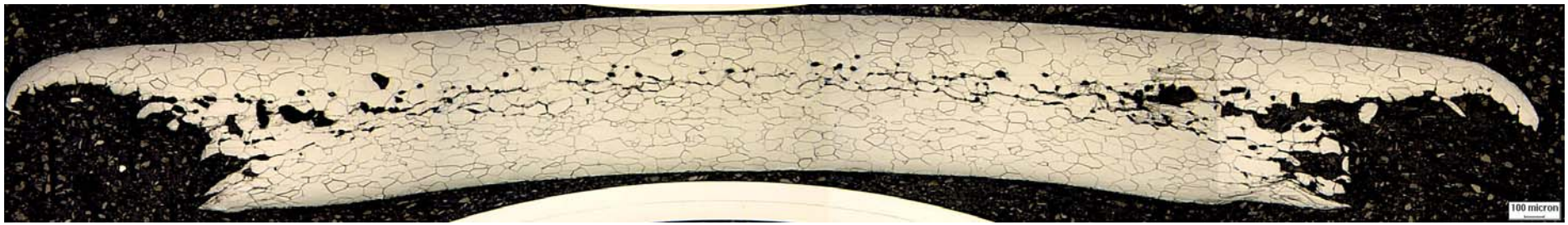


The ductile failure process in polycrystalline metals generally involves porosity initiation, porosity growth / coalescence and localized deformation in various combinations dependent upon material type and boundary conditions.

Los Alamos NATIONAL LABORATORY EST.1943

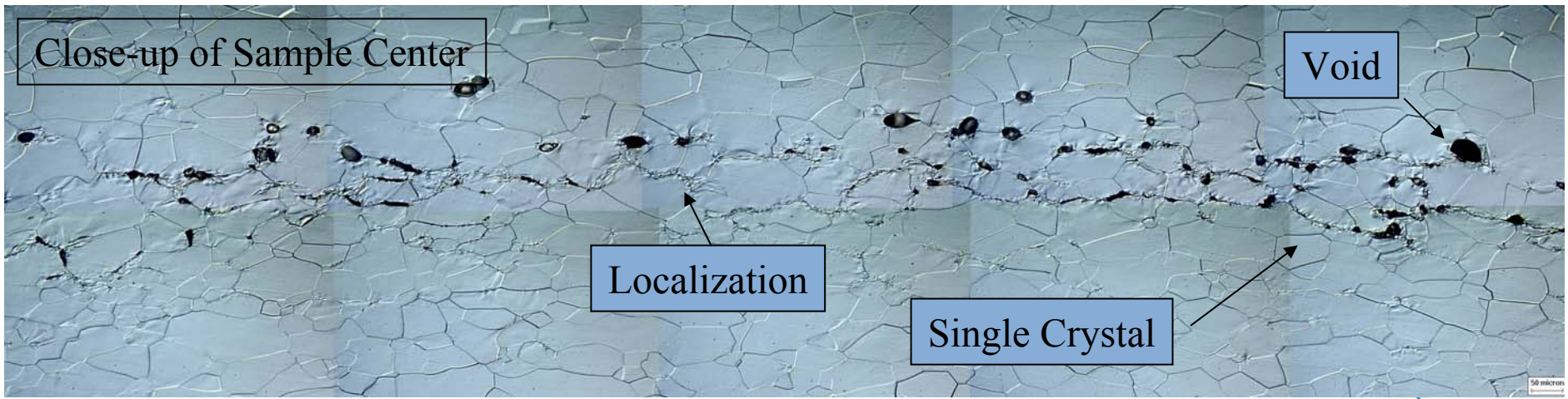
ASC™

Explosively Loaded Sample Demonstrates Ductile Damage and Failure Physics



T. Mason

Explosively Loaded Tantalum Experiment
6 mm thick PETN Underneath Sample – Center Detonated
Soft Sample Recovery



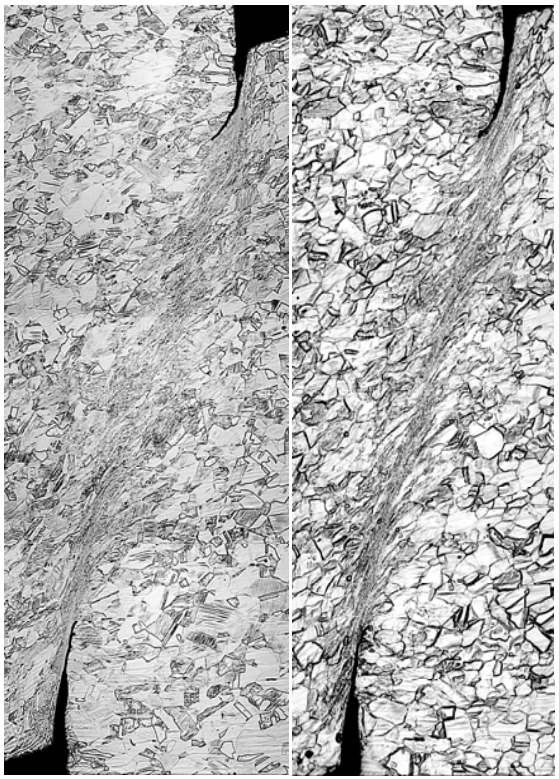
'Void sheets' are forming along strain localizations in sample

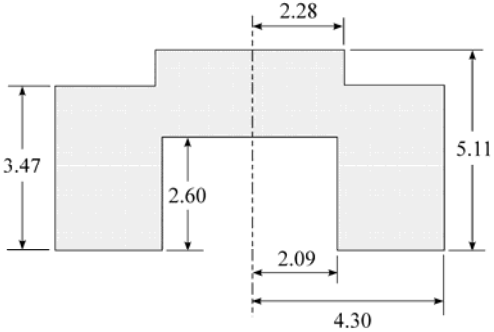
Los Alamos NATIONAL LABORATORY EST.1943

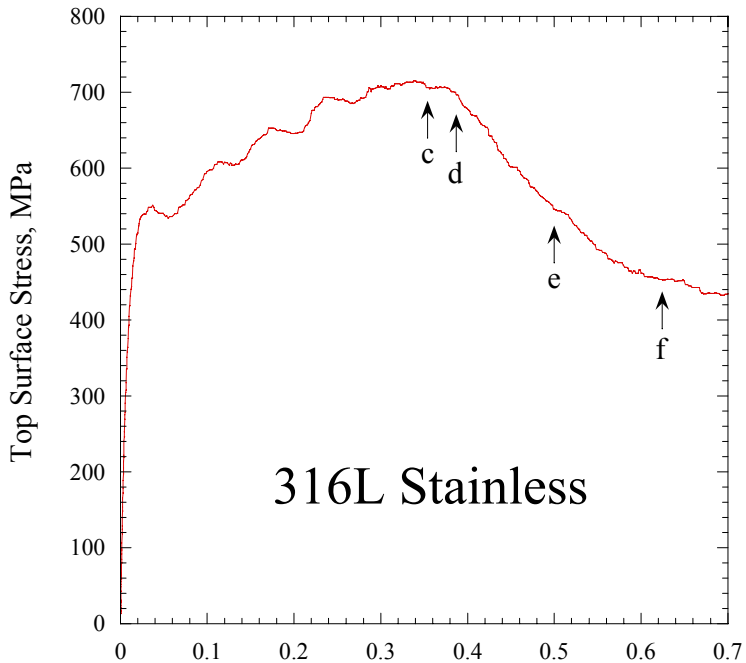
ASC™

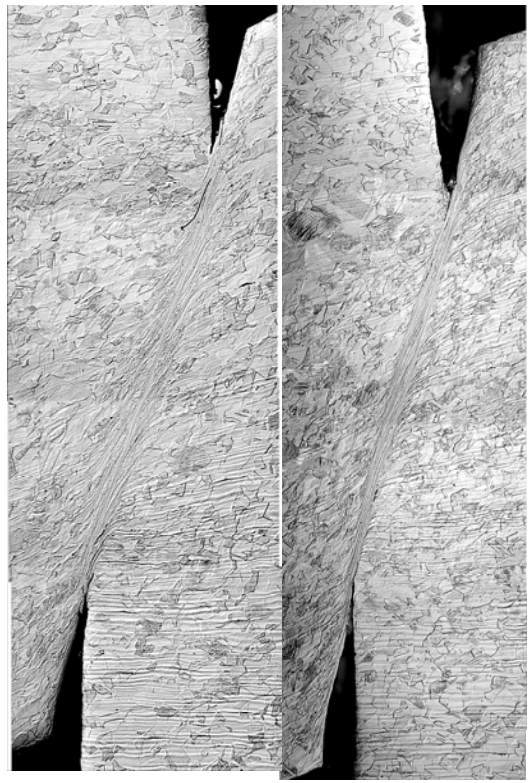
Some Ductile Materials Choose to Fail by Formation of Adiabatic Shear Bands

Q. Xue









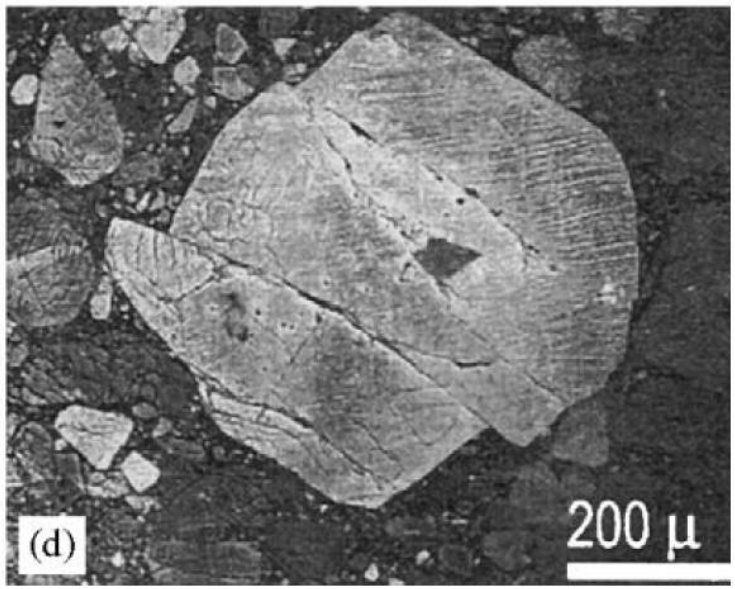
C D E F

Ductile Behavior

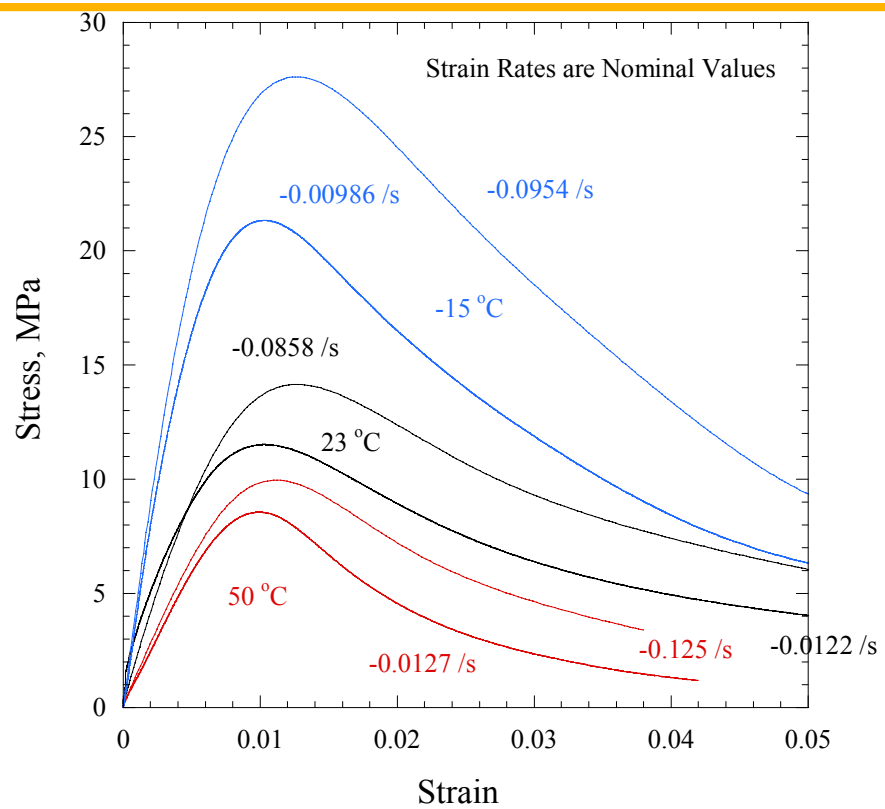
- The ductile failure process in polycrystalline metals generally involves porosity initiation, porosity growth / coalescence and localized deformation in various combinations dependent upon material type and boundary conditions.
- Polycrystalline metals are inhomogeneous aggregates which produce inhomogeneous deformation fields. The ductile failure process is heavily dependent upon the existence of inclusions. How do we model this stochastic process in a computationally efficient manner?
- Many materials experience phase changes during the deformation process (inhomogeneously within grains). How does this impact the damage and failure process?
- Traditionally we have relied on deviator based plasticity models and have handled pressure modeling through the use of equations of state – how good is this approach at high rates of loading where pressures can be very large?

Brittle Behavior

PBX 9501, D. Thomson

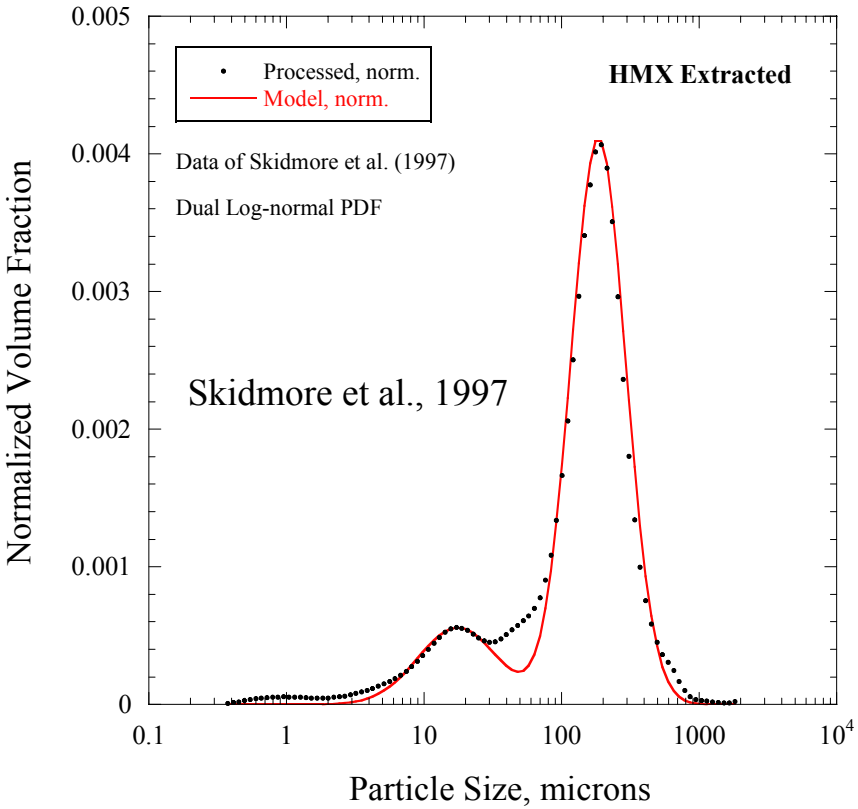


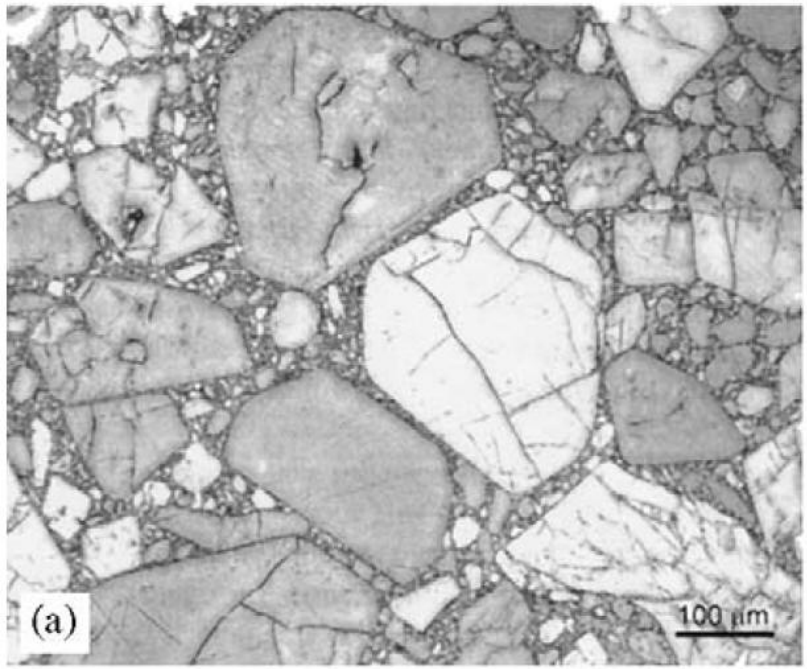
HMX, J. Dienes et al., 2006



Brittle behavior is characterized by mixed mode fracture processes which begin at the micro-scale but can propagate to the macro-scale. Brittle behaved phases (materials) are often combined with ductile phases (materials) in the aggregate.

There is also interest in Microstructural Characterization





HMX, J. Dienes et al., 2006

In order to model and predict the statistics of the ductile damage and failure process, one must also quantify and represent the statistical character of the aggregate microstructure.

Los Alamos NATIONAL LABORATORY EST.1943

ASC™

Brittle Behavior

- As in the example of PBX 9501, brittle and ductile polycrystalline phase aggregates are of strong interest for explosives and metallic polycrystalline materials. This is a complicated extension of the ductile damage process producing an even more heterogeneous response. How do we model this stochastic process in a computationally efficient manner?
- Mixed-mode fracture under general dynamic loading conditions. How do we track history effects for complex loading paths when new surfaces are created? Do cleavage processes follow the same close-packed rules as slip processes in plasticity?
- Brittle damage processes occur at relatively small strains in comparison to ductile damage processes, yet our interest is inherently in large strain behavior. When do fracture based processes of brittle behavior give way to granular flow processes?
- Are particle based computational frameworks more appropriate than finite element or finite difference based codes for these problems with severe discontinuities?

Multi-Length Scale Problem

Macro-Mechanical

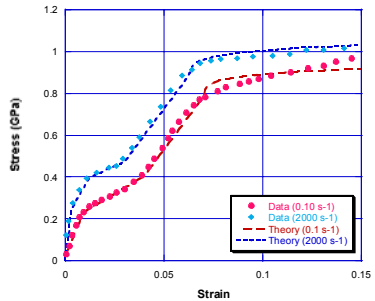
Polycrystal

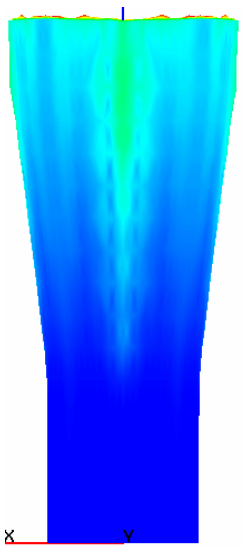
Single Crystal

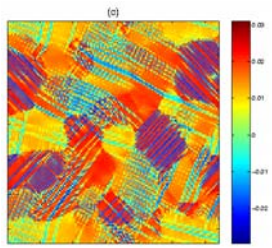
Molecular Dynamics

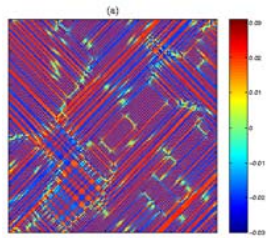
Quantum Mechanics

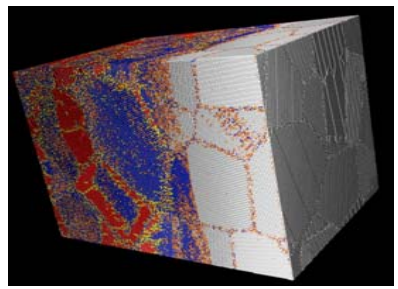
Experiment

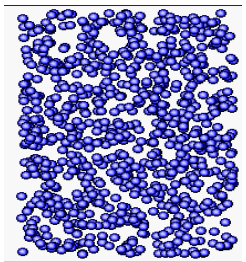












Time / Length Scales

Los Alamos NATIONAL LABORATORY EST.1943

ASC™

Multi-Length Scale Problem

- The physics of damage initiation and growth is inherently a small scale process. The multi-length scale problem is of continued interest.
- We are also interested in seeing research programs which are well balanced in experimental and theoretical/computational work. Development of small-scale experimental techniques in tandem with small-scale computational work.
- The damage and failure process in polycrystalline materials is stochastic. How does one represent these statistics computationally without resorting to direct simulations?
- Although linking of multi-scale physics using concurrent modeling strategies is interesting, we are most interested in strategies for bridging length scales by more computationally efficient means.
- The desire is to have the ASC Alliance Centers work more closely with staff from the national laboratories in the future. This is a shared responsibility.